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Toward Paradoxical Inconsistency in Electrostatics of Metallic Conductors

by Michael Grinfeld and Steven B Segletes

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Weapons and Materials Research Directorate, ARL

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authors' email: <michael.greenfield4.civ@mail.mil>, <steven.b.segletes.civ@mail.mil>.

14. ABSTRACT
Current developments show a clear trend toward more serious efforts in validation and verification (V&V) of physical and engineering models. Naturally, when dealing with fundamental problems, the V&V effort should include careful exploration and, if necessary, revision of the fundamentals underlying the physics. With this understanding in mind, we review some fundamentals of the models of crystalline electric conductors and find a significant inconsistency in applying classical electrostatics to these sorts of substances. In this report, we formulate this inconsistency in the form of a novel paradox in electrostatics of metallic conductors.

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1. Introduction: Why Electrostatics?

With so many advanced methods and computational techniques available, why are we to focus here on classical electrostatics as a means to describe the charge distribution in a body? Quantum methods give a deeper picture at the atomic level and computational methods are very accurate for these types of problems.

However, the analytical solutions afforded by classical electrostatics, unavailable to the more computationally driven disciplines, provide a powerful tool for both understanding the macroscopic picture, as well as providing exact solutions against which developing computational methods may be verified. The importance of this latter point cannot be overstated.

The fact that classical electrostatics is still widely employed by engineering practitioners, both directly as well as under the pretext of their computer-packaged models, indicates that it is still a relevant method. If an inconsistency can be shown in the classical theory for a certain class of problems, then understanding the nature and scope of this inconsistency is vital for initially avoiding and, eventually, resolving the issue. In this report, we draw attention to such an inconsistency, which arises when the classical method is applied to a crystalline-solid conductor.

This inconsistency is very relevant to the underpinning of the large-scale computational methods employed in our laboratory, in which magneto-hydrodynamic (MHD) models, originally developed for "fluid" systems (the "hydro" in "hydrodynamic") are being applied to systems composed of crystalline-metallic bodies. Just as the solid mechanics extentions to hydrodynamic modeling (such as strength, plasticity, and fracture) required and continue to require much development from many quarters, so too do the more recent MHD models require verification and development, as the scope of their application extends from the realm of fluids into that of solids.

2. Classical Electrostatics of Conductors

The great Niels Bohr permanently insisted on the crucial role of paradoxes in scientific progress. His famous quotes are posted on the Internet: "How wonderful that we found a paradox. Now, we have a chance to make progress" and, even more eloquent, "No paradox – no progress!" Developing paradoxes regarding the fundamentals never becomes old or obsolete. Moreover, they are the strongest triggers of a subsequent conceptual growth of the corresponding discipline. This is why we

formulate within this report a novel paradox, which we faced when modeling a solid (crystalline) conductor.

Consider an isolated piece Ω of a crystalline charged conductor carrying a total charge Q. According to the classical model of electrostatics, this charge will be distributed along the smooth boundary Σ of the domain Ω with the surface density σ (Fig. 1). In the case of a spherical domain Ω with radius R, the spherical symmetry of the problem implies that the surface density will be uniform: $\sigma = 3Q/4\pi R^3$, and the field $\vec{E}$ at the distance r from the center of the sphere will be directed radially with an absolute value equal to $|Q|/r^2$.
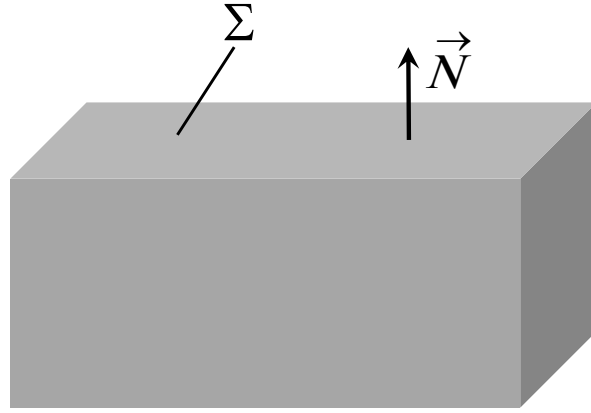
Fig. 1 An isolated domain Ω of an electric conductor

If the finite domain Ω deviates from spherical shape, the density σ will be different at the different points of the boundary Σ. To find the function σ, one has to solve the boundary value problem with respect to the function σ and the electrostatic potential φ, which reads (see, for instance, Stratton[1] and Landau and Lifshitz[2]):

1) Outside the domain Ω

$$\nabla^i \nabla_i \varphi = 0 \quad . \tag{1}$$

2) The potential is equal to a constant φ° at the surface Σ:

$$\varphi|_\Sigma = \varphi^\circ \quad . \tag{2}$$

3) The normal component of the potential gradient at Σ and surface density σ are

connected by the relationship

$$N^i \nabla_i \varphi \big|_{\Sigma_+} = -4\pi\sigma \quad . \tag{3}$$

4) The potential decays to 0 at infinity:

$$\lim_{|\vec{z}| \to \infty} \varphi = 0 \quad . \tag{4}$$

5) The total charge should be equal to Q:

$$\int_{\Sigma} d\Sigma\sigma = Q \quad . \tag{5}$$

Symbol Σ_+ in boundary condition 3 means that the limit should be taken when approaching the boundary from the outside of the crystal (it is easy to figure out that same limit from the inside vanishes because there is no electrostatic field inside a conductor.)

Only for a few simple shapes does the boundary value problem defined by Eqs. 1–5 permit explicit solutions. Even in the relatively simple case of a triaxial ellipsoid, the explicit solution expresses in terms of elliptic integrals. Advances in computational platforms allow for calculations of solutions for quite sophisticated conductor shapes.

3. Models of Conductors

Scholars realized centuries ago that there are 2 sorts of electricity, involving negative and positive charges.[3] In the first models, they were treated as 2 similar liquids. The idea of liquid came from the fact that charges were able to move between the bodies. There was not enough understanding to make a clear distinction between the physical properties of these 2 electric liquids. Therefore, intuitively, they were treated the same way with respect to any physical properties except for the signs of the charges. This similarity is reflected in the master system of electrostatics, Eqs. 1–5. This system is the same for positive and negative charges.[*]

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[*]Of course, despite its aesthetic beauty, classical electrostatics has multiple weaknesses. For instance, when talking about the surface density of charges, we tacitly assume that the charged liquids have infinite compressibility since their 3-D volume is equal to 0. We do not discuss here these

Later on, much more elaborate models of conductors appeared, including models of solid conductors. What we intend to discuss here is the paradoxical inconsistency of the classical electrostatic theory with respect to solid conductors.

The classical model of a crystalline conductor consists of material composed of a lattice of positively charged ions (Fig. 2). We interpret the term "lattice" to imply that the ions are rigidly attached to the coordinates of the associated body. Basically, these ions cannot change relative position with respect to each other (aside from atomic vibrational oscillations) and, thus, the spatial density of positive charges can be reliably assumed fixed. In the conductor, the situation is different with the negative charges of electrons. A relatively small fraction of electrons (the outer-shell valence electrons) are free to move along and within the whole conductor (unlike the positive ions, which are constrained to merely oscillate about their respective equilibrium positions). These unbound electrons (and only these) are able to move freely through the conductor and, thus, can be treated as an electron liquid.
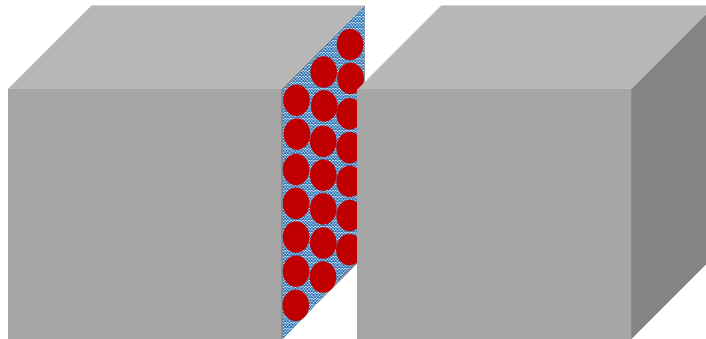
Fig. 2 Cutaway view of a crystalline conductor

Since the electrostatic forces are extremely large (contrary to, say, gravitational forces), charges of opposite sign try to annihilate the influence of each other by creating macro-domains with a zero net electrostatic charge. Thus, according to the classical theory, all the internal regions of the conductor appear to be macroscopically charge-neutral, and when there is an excess charge of one of the signs, the noncompensated charge concentrates at the conductor's boundary.

weaknesses—they are not the topic of this report. After all, classical electrostatics works perfectly well in multiple instances of practical importance. For example, plasma of ionized gases, in many respects, can be described by the model of 2 oppositely charged liquids.

4. Paradoxical Inconsistency between the Classical Model of Electrostatics and the Model of Crystalline Conductors

Where is the inconsistency between the electrostatics system, Eqs. 1–5, and the above-mentioned model of crystalline conductors? It is this: the electrostatic system, given by Eqs. 1–5, treats equally the cases of macroscopic excess of positive or negative charges Q. In fact, the positively charged ions are "nailed" to the lattice (if we neglect their nanoscale oscillations in the vicinity of their equilibrium positions). In particular, the macroscopic density q_+ per unit volume of the positively charged ions cannot change and remains constant. The situation with negative charges of the electrons is different, since part of them—the unbound electrons, can move freely and change arbitrarily the volumetric density q_- of negative charge. The net charge density q_{net} per unit volume is defined as

$$q_{net} \equiv q_+ + q_- \quad . \tag{6}$$

It is this very charge density q_{net} that produces the macroscopic electric field (the macroscopic electric effect should be distinguished from the microscopic electromagnetic field, which attains many orders of magnitude higher values in the close proximity of electrons and ions).

In this model of a crystalline conductor, therefore, the net charge density q_{net} cannot assume positive values that exceed its maximum value q_+. At the same time, $|q_-|$ can assume arbitrarily large values due to the unlimited mobility of unbound electrons. Thus, in contrast, the macroscopic charge density q_{net} can assume unlimited negative values, but only finite positive values q_+.

This point is illustrated in Fig. 3, depicting excess charge upon a crystalline sphere. In Fig. 3a, for the case of excess negative charge, the mobility of the free electrons allows the excess charge to be concentrated in a surface layer of thickness ϵ, where the value of ϵ can be idealized to approach zero, in accordance with the theory of electrostatics. As $\epsilon \to 0$, the volumetric density of electrons will become unbounded. On the other hand, in Fig. 3b, when there is an excess of positive ions (due to the removal of free electrons), the layer containing positive ions, of thickness ϵ, cannot approach zero thickness under idealization, because the lattice fixes the ions in place—they are not free to move to achieve a denser volumetric concentration. The volumetric density of the positive charge, therefore, cannot exceed a value of

the valence charge per unit cell volume.[*]
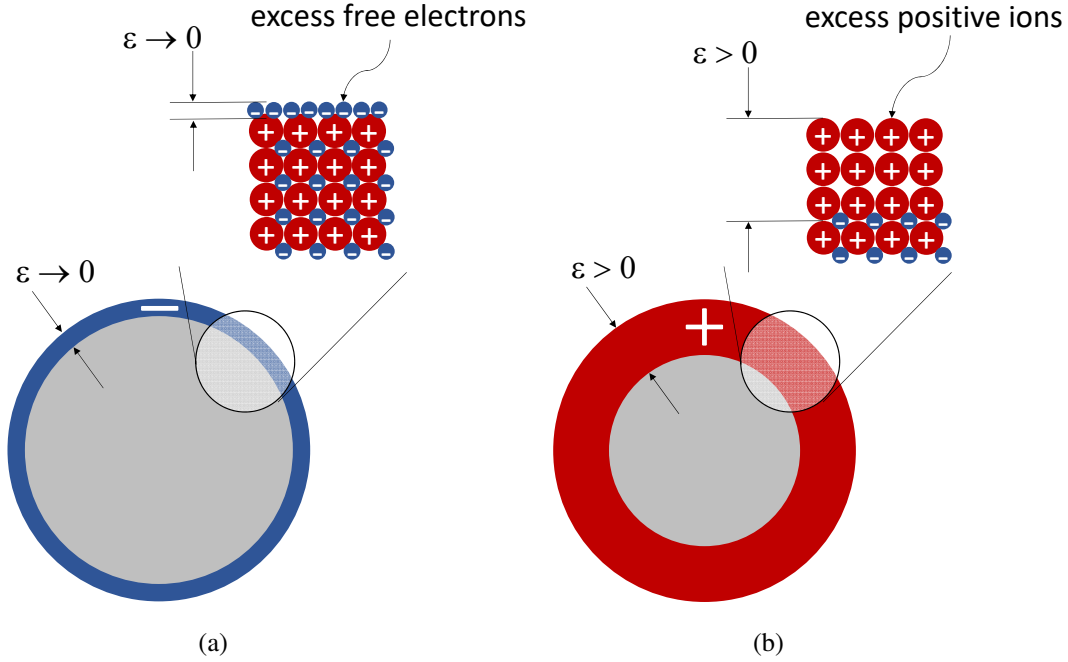
Fig. 3 Cases of a charged crystalline sphere, with (a) excess negative charge and (b) excess positive charge. Note that the color gray indicates electrically neutral conductor, blue a surface layer of electrons, and red a lattice of (net) positive ions.

The electrostatics master system, Eqs. 1–5, can be solved for positive or negative values of Q. In particular, in the case of a spherical conductor, we get the surface density σ equal to $\sigma = 3Q/4\pi R^3$. When Q is negative, the corresponding value of the surface charge density σ is negative. In other words, in the vicinity of the conductor's boundary, the 3-D density of electrons is infinite. Although, in the ultimate physical theory, nothing should be infinite, this conclusion is consistent with our model of the conductor. Indeed, due to the unconstrained mobility of electrons, their 3-D density can be arbitrarily large. But when Q is positive, we arrive at the positive surface density σ of the net charge. Thus, per this solution of classical electrostatics, the 3-D density of the positive charge should be able to assume arbitrarily large positive values. But this conclusion is incompatible with our crystalline model, since the 3-D net charge density cannot exceed the value of q_+ in the lattice. This contradiction is the essence of our paradox of classical electrostatics of crystalline conductors: that the respective cases of excess negative and excess positive

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[*]Quantitative estimations of this maximum positive charge density, characterized by q_+, may be imported from various atomic methods, such as quantum mechanics.

charge in the same crystalline body result in different net charge distributions of the excess charge, violating the governing principle of classical electrostatics.

5. Conclusion

In this report, we draw the reader's attention to the inconsistency of classical electrostatics of conductors, using the concept of the finite nonvanishing surface density of electric charge. The classical electrostatics model implies that the 3-D density of positive charges can grow without limit by macroscopic migration of positive charges. In fact, only very mobile negative charges, unbound electrons, have such an ability. The positive charges are "nailed" to the crystalline lattice. Thus, they, basically, have an unchangeable finite 3-D density and zero surface density. This inconsistency between the classical electrostatics and classical model of a crystalline conductor should be eliminated. To that end, an essential revision of the system of classical electrostatics of crystalline conductors seems unavoidable.

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